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Complex formation between 1,1,1,3,3,3-hexafluoro-2-propanol and dimethyl ether verified by FTIR spectroscopic measurements and ab initio calculations.

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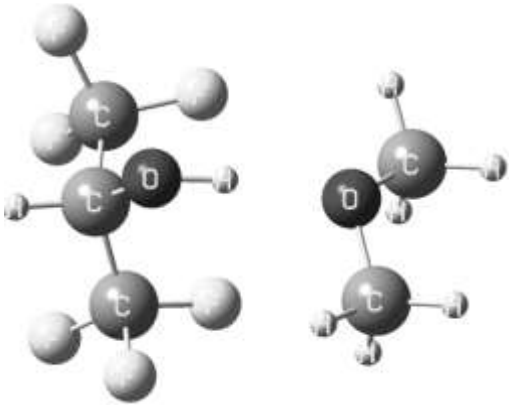
Halogenated alcohols, specifically 1,1,1,3,3,3-hexafluoro-2-propanol (HFIP) are one of the model systems which might reveal anesthetic potency. One of possible mechanisms of anesthetic effect refers to non-covalent interactions between these compounds and a target. It is also worth to note that HFIP is the basic product of metabolism of sevoflurane which is widely used as an effective, relatively harmless inhalation anesthetic. In the present study, features of complex formation between HFIP and dimethyl ether (DME) are examined by the help of FTIR spectroscopy and ab initio calculations. The results obtained suggest HFIP/DME complex formation stabilized by H – bond of OH…O type. This heterodimer is additionally stabilized by weaker van der Waals contacts between F atoms of the alcohol and hydrogen atoms of the ether. At room temperature, both conformers of HFIP (antiperiplanar (ap) and synclinal (+-sc)) participate noticeably in complex formation. Results of calculations performed at MP2 level with correlation consistent basis sets augmented by diffuse functions are in line with experimental observations.



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